N,N-Dimethylformamide 68-12-2 | DTXSID6020515

Model Performance

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Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 150 °C

Global applicability domain: Inside

Local applicability domain index: 6.43e-01

Confidence level: 7.34e-01

Nearest Neighbors from the Training Set

Image not found

N,N-Dimethylformamide

Measured: 153 Predicted: 150

Image not found

N,N-Dimethylacetamide

Measured: 165 Predicted: 168

Image not found

Chloroacetonitrile

Measured: 126 Predicted: 126

Image not found

Acetonitrile, methoxy-

Measured: 119 Predicted: 130

Image not found

3-Chloropropionitrile

Measured: 176 Predicted: 157